Numerically Accurate *GW* Approach to Electronic Band Structure of Weakly and Strongly Correlated Materials

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Abstract:
Many-body perturbation theory in the *GW* approximation is currently regarded as the most accurate and robust first-principles approach to determine electronic band structure of weakly correlated insulating materials without any empirical input. Recent systematic studies of ZnO by several groups clearly indicate the importance of numerical accuracy in the practical implementation of the *GW* methods. In this talk I will address the challenges for numerically accurate *GW* calculation based on our recent systematic investigation of the effects of including high-energy local orbitals (HLOs) in the linearized augmented plane waves (LAPW)-based *GW* calculations for both weakly and strongly correlated materials [1-3]. It is shown that both the accuracy of unoccupied states and the completeness in the summation of states are crucial for numerically accurate *GW* calculations. In general, using LAPW+HLOs basis can significantly improve the performances of the semi-local density functional approximation based GW_0 approach [2]. We have further investigated other systems with electronic configurations that are significantly different from those of common sp semiconductors, including VII-IB compounds (MX with M=Cu, Ag and X=Cl, Br and I) and strongly correlated d- or f-electron oxides (NiO, Ce_2O_3 and UO_2) [3]. We found that the consideration of HLOs in the *GW* based on density-functional theory plus the Hubbard *U* correction (GW_0@DFT+U) approach can significantly improve the description of electronic band structure of those d- and f-electron systems.

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[2] H. Jiang and P. Blaha, Phys. Rev. B, **93**, 115203(2016).
[3] H. Jiang, Phys. Rev. B, **97**, 245132(2018).